Claims

1.   A method of characterizing a molecule for determining molecular similarity or diversity including:

determining intramolecular distances between atoms of the molecule to

5   characterize a shape of the molecule; and

for each of a group of properties, determining intramolecular distances between atoms with that property and other atoms of the molecule.

2.   The method of claim 1, further comprising:

sorting distances by magnitude to create a curve;

10   numerically characterizing the curve; and

storing values representing the numerical characterization of the curve.

3.   The method of claim 1, wherein the atoms that are used are heavy, non-hydrogen atoms.

4.   The method of claim 1, wherein the atoms with a property are acidic

15   atoms.

5.   The method of claim 1, wherein the atoms with a property are basic atoms.

6.   The method of claim 1, wherein the atoms with a property bear a formal positive charge.

20   7.   The method of claim 1, wherein the atoms with a property bear a formal negative charge.

8.   The method of claim 1, wherein the atoms with a property bear a partial positive charge.

9.   The method of claim 1, wherein the atoms with a property bear a

25   partial negative charge.

10.   The method of claim 1, wherein the atoms with a property are hydrophobic atoms.

11.   The method of claim 1, wherein the atoms with a property are polarizable atoms.

12.   The method of claim 1, wherein the atoms with a property are hydrogen-bond donor atoms.

13.   The method of claim 1, wherein the atoms with a property are hydrogen-bond acceptor atoms.

14.   The method of claim 1, wherein the atoms with a property are aromatic atoms.

15.   The method of claim 1, wherein the atoms with a property are all atoms.

16.   The method of claim 1, wherein the method is performed for a number of molecules to create a series of fingerprints and the fingerprints are stored in a database.

17.   The method of claim 16, wherein the fingerprints are compared on a pairwise basis to determine relative similarities to each other.

18.   The method of claim 16, wherein in response to a determination that a molecule is desired with a particular shape and/or one or more properties, the method further comprising searching the fingerprints in the database to identify a molecule that has the desired shape and/or properties.

19.   The method of claim 2, wherein the method is performed for a number of molecules to create a series of fingerprints and the fingerprints are stored in a database.

20. The method of claim 19, wherein the fingerprints are compared on a pairwise basis to determine relative similarities to each other.

21. The method of claim 19, wherein in response to a determination that a molecule is desired with a particular shape and/or one or more properties, the method further comprising searching the fingerprints in the database to identify a molecule that has the desired shape and/or properties.

22. The method of claim 16, further comprising searching the fingerprints to determine one or more molecules likely to bind to another molecule.

23. The method of claim 22, wherein said another molecule is a protein.

24. The method of claim 16, further comprising grouping together fingerprints considered sufficiently similar.

25. The method of claim 16, further comprising using a fingerprint to predict the binding ability of the molecule associated with that fingerprint to another molecule, as compared to the binding ability of another known molecule.

26. A method of characterizing a molecule for determining molecular similarity or diversity including:

determining intramolecular distances between atoms of the molecule to characterize a shape of the molecule;

sorting the distances to create a curve;

numerically characterizing the curve; and

storing values representing the numerical characterization of the curve and therefore of the molecule.

27. A method of characterizing a molecule for determining molecular similarity or diversity including:

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for each of a group of properties, determining intramolecular distances between atoms with that property and other atoms of the molecule;

sorting the distances to create a curve;

numerically characterizing the curve; and

storing values representing the numerical characterization of the curve and therefore of the molecule.

28.   The method of claim 27, wherein the property includes one or more of the following: acidic moieties, basic moieties, moieties of formal positive charge, moieties of formal negative charge, moieties of partial positive charge, moieties of partial negative charge, hydrophobic moieties, polarizable moieties, hydrogen-bond donor moieties, hydrogen-bond acceptor moieties, and aromatic moieties.